Methods for Scaling to Doubly Stochastic Form*

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ABSTRACT

New methods for scaling square, nonnegative matrices to doubly stochastic form are described. A generalized version of the convergence theorem of Sinkhorn and Knopp (1967) is proved and applied to show convergence for these new methods. Tests indicate that one of the new methods has significantly better average and worst-case behavior than the Sinkhorn-Knopp method; for one of the 3×3 examples of Marshall and Olkin (1968), SK requires 130 times as many operations as the new algorithm to achieve row and column sums 1 ± 10^{-5}.

1. INTRODUCTION

We seek an algorithm which will find a pair of positive diagonal matrices D and E for a given square nonnegative matrix A, such that DAE is doubly stochastic—or determine that such a pair does not exist.

A nonnegative $n\times n$ matrix A is said to have *support* if it possesses a positive diagonal; A has *total support* if $A\neq0$ and every positive entry in A

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lies on a positive diagonal. A is *fully indecomposable* if it is impossible to find permutation matrices P and Q so that

$$PAQ = \begin{pmatrix} A_1 & 0 \\ A_2 & A_3 \end{pmatrix} \tag{1.1}$$

with A_1 square.

Three procedures for computing D and E, when they exist, have appeared in the literature:

(1) minimize x^tAy subject to the constraints $\prod x_i = \prod y_i = 1$,
(2) minimize

$$f(x_1,\dots,x_n) = \frac{\prod_{k=1}^{n}\left(\sum_{i=1}^{n} a_{ki}x_i\right)}{\prod_{k=1}^{n} x_k}$$

subject to the constraints

$$x_k > 0, \quad k = 1,\dots,n, \quad \text{and} \quad \sum_{k=1}^{n} x_k = 1,$$

and

(3) compute D and E iteratively by alternately normalizing all rows and all columns in A. The first method is due to Marshall and Olkin [10]; the second is described by Djokvic [6]. In each case, the minimization problem is shown to have a solution when A is fully indecomposable. The third algorithm was first described by Deming and Stephan [5], who called it the "iterative proportional fitting procedure." It was rediscovered by Sinkhorn [14–17], and Sinkhorn and Knopp [18] proved that D and E exist such that DAE is doubly stochastic if and only if A possesses total support. Further, they showed that in such a case, the iteration converges to a solution pair D and E. Brualdi, Parter, and Schneider [4] independently proved the existence of D and E when A is a direct sum of fully indecomposable matrices by showing that its corresponding Menon operator [12] has a fixed point. Finally, Sinkhorn [15] showed that the Sinkhorn-Knopp method converges geometrically for positive starting matrices.

The following result can be applied to show that a nonnegative matrix has total support if and only if it is a direct sum of fully indecomposable matrices:

FROBENIUS-KONIG THEOREM [9, p. 97]. *A nonnegative $n \times n$ matrix without support contains an $s \times t$ zero submatrix, where*

$$s + t = n + 1.$$

In this paper we describe three new iterative procedures for scaling nonnegative matrices to doubly stochastic form. We prove a generalized version of the convergence theorem in [18] and apply it to show that for starting matrices with total support, these new iterations converge to diagonally equivalent limits which are multiples of doubly stochastic matrices. In the final—and (to us) most interesting—section, we present results of tests comparing our new methods with the Sinkhorn-Knopp method (SK). One of the new algorithms, EQ, exhibited significantly better average and worst-case behavior than SK: for some test matrices, SK required 130 times as many operations as EQ (where an operation is a multiply or a divide), and examples for which EQ requires more than ten times as many operations as SK are rare.

We wish to mention that all the methods we discuss are easy to implement. Our methods do some analysis and then choose a row and/or column to be modified. Consequently the logic in the programs is more complicated than in Sinkhorn and Knopp's. Nevertheless EQ requires only 200 executable FORTRAN statements.

Techniques for scaling to doubly stochastic form have a number of applications. The problem that launched Sinkhorn's research was estimating the transition matrix in a Markov chain. Marshall and Olkin [11] give references to other statistical applications. They can be applied to equilibrate a general matrix with respect to any p-norm, $p \neq \infty$; one of us has used EQ to test for diagonal equivalence to orthogonal form by equilibrating with respect to the 2-norm. Finally, we remark that doubly stochastic matrices possess the following interesting properties:

(1) they are "perfectly balanced" with respect to the 1-norm [13];

(2) their p-norms are unity for all $p \leqslant \infty$ [20]; and

(3) their inverses—if they exist—have row and column sums equal to unity (though the inverse of a doubly stochastic matrix is doubly stochastic only for permutation matrices).

2. ALGORITHMS

In this section, we will describe three iterative procedures for scaling nonnegative matrices to doubly stochastic form. In Section 3 we show that when they are applied to a matrix with total support, the result is a sequence of iteration matrices converging to a multiple of a doubly stochastic matrix.

Our first algorithm, DEV, was motivated by the desire to have an algorithm that would modify a single row or column—leaving the remainder of the matrix unchanged—at each iterative step. There is a natural way to select the row or column to be changed: choose one whose sum deviates maximally from the mean of the row sums (which is also the mean of the column sums). This approach is reasonable, because matrices with equal row and column sums are scalar multiples of doubly stochastic matrices. For the same reason, the natural change is to multiply entries in the selected row or column by a factor chosen so that its new sum will be the new mean of row sums.

ALGORITHM 1 (called DEV, for deviation reduction). Given $A = A^{(0)}$, an $n \times n$ matrix:

(1) Compute row and column sums for A:

$$r_i \leftarrow \sum_{j=1}^{n} a_{ij}, \qquad i = 1, \dots, n,$$

$$c_j \leftarrow \sum_{i=1}^{n} a_{ij}, \qquad j = 1, \dots, n.$$

Compute the mean, μ, of row sums in A:

$$\mu \leftarrow \frac{1}{n}\left(\sum_{i=1}^{n} r_i\right).$$

(2) Find indices p and q so that

$$|r_p - \mu| = \max_i |r_i - \mu|$$

and

$$|c_q - \mu| = \max_j |c_j - \mu|.$$

If $|r_p - \mu| < \mathrm{tol}\cdot\mu$ and $|c_q - \mu| < \mathrm{tol}\cdot\mu$ go to step 5. If $|c_q - \mu| > |r_p - \mu|$ go to step 4.

(3) Calculate the mean $\bar{\mu}$ of row sums other than r_p:

$$\bar{\mu} \leftarrow \frac{1}{n-1}\left(\sum_{\substack{i=1\\i\neq p}}^{n} r_i\right).$$

Scale row p to $\bar{\mu}$:

$$a_{pj} \leftarrow a_{pj}\frac{\bar{\mu}}{r_p}, \qquad j=1,\ldots,n.$$

Update row and column sums for A:

$$r_p \leftarrow \bar{\mu},$$

$$c_j \leftarrow c_j + \left(\frac{\bar{\mu}}{r_p} - 1\right)a_{pj}, \qquad j=1,\ldots,n.$$

Go to step 2.

(4) Calculate the mean, $\bar{\mu}$, of column sums other than c_q:

$$\bar{\mu} \leftarrow \frac{1}{n-1}\left(\sum_{\substack{j=1\\j\neq q}}^{n} c_j\right)$$

Scale column q to $\bar{\mu}$:

$$a_{iq} \leftarrow a_{iq}\frac{\bar{\mu}}{c_q}, \qquad i=1,\ldots,n.$$

Update row and column sums for A:

$$c_q \leftarrow \bar{\mu}$$

$$r_i \leftarrow r_i + \left(\frac{\bar{\mu}}{c_q} - 1\right)a_{iq}.$$

Go to step 2.

(5) Normalize:

$$a_{ij} \leftarrow \frac{1}{\mu} a_{ij}, \qquad i, j = 1, \ldots, n.$$

Exit.

REMARKS. Note that step 3 is equivalent to premultiplying the matrix A by a positive diagonal matrix:

$$D = \operatorname{diag}(d_1, \ldots, d_n),$$

where

$$d_i = \begin{cases} 1 & \text{if } i \neq p, \\ \mu / r_p & \text{if } i = p, \end{cases}$$

and step 4 is equivalent to postmultiplying the matrix A by a positive diagonal matrix:

$$E = \operatorname{diag}(e_1, \ldots, e_n)$$

where

$$e_j = \begin{cases} 1 & \text{if } j \neq q, \\ \bar{\mu} / c_q & \text{if } j = q. \end{cases}$$

We say that a row and column pair in a nonnegative matrix is *balanced* (with respect to the 1-norm) if they have equal sums. Obviously, all row and column sums in a multiple of a doubly stochastic matrix are balanced. A second approach to scaling to doubly stochastic form, then, is to find a row and a column whose sums have maximal difference and to scale the matrix so that their sums are equal. This is the approach taken by our second algorithm.

ALGORITHM 2 (called BAL, for balance). Given $A = A^{(0)}$, an $n \times n$ nonnegative matrix:

(1) Compute row and column sums for A:

$$r_i \leftarrow \sum_{j=1}^{n} a_{ij}, \qquad i = 1, \ldots, n,$$

$$c_j \leftarrow \sum_{i=1}^{n} a_{ij}, \qquad j = 1, \ldots, n,$$

and the mean of row sums:

$$\mu \leftarrow \frac{1}{n} \left(\sum_{i=1}^{n} r_i \right).$$

(2) Find indices p and q so that

$$|r_p - c_q| = \max_{i,j} |r_i - c_j|.$$

If $|r_p - c_q| < \mu \cdot \mathrm{tol}$ go to step 5.
(3) Balance row p and column q: Multiply entries in row p by

$$f = \left(\frac{c_q - a_{pq}}{r_p - a_{pq}} \right)^{1/2},$$

and multiply entries in column q by f^{-1}.
(4) Update row and column sums:

$$\begin{aligned}
r_i &\leftarrow r_i + (f^{-1} - 1)a_{iq}, \qquad i = 1,\ldots,n,\\
r_p &\leftarrow \{(r_p - a_{pq})(c_q - a_{pq})\}^{1/2} + a_{pq},\\
c_q &\leftarrow r_p,\\
c_j &\leftarrow c_j + (f-1)a_{pj}, \qquad j = 1,\ldots,n,\\
\mu &\leftarrow \frac{1}{n}\sum_{i=1}^{n} r_i.
\end{aligned}$$

Go to step 2.
(5) Normalize:

$$a_{ij} \leftarrow \frac{1}{\mu} a_{ij}, \qquad i,j = 1,\ldots,n.$$

Exit.

Note that step 3 is equivalent to forming the product DAE, where

$$\begin{aligned}
D &= \mathrm{diag}(d_1,\ldots,d_n),\\
d_i &= \begin{cases} 1 & \text{if } i \neq p,\\ f & \text{if } i = p, \end{cases}\\
E &= \mathrm{diag}(e_1,\ldots,e_n),\\
e_j &= \begin{cases} 1 & \text{if } j \neq q,\\ f^{-1} & \text{if } j = q. \end{cases}
\end{aligned}$$

Now for the third method. When testing DEV we found cases where a sequence of 10 or more iterations were alternately scaling the same row and the same column. Our third algorithm is a variant of DEV that avoids this problem. It records the last row and last column scaled; when it detects a repeat, it performs a balancing step.

ALGORITHM 3 (called EQ, for equalize). Given $A = A^{(0)}$, an $n \times n$ non-negative matrix:

(1) Initialize:

$$\text{lastr} \leftarrow 0,$$

$$\text{lastc} \leftarrow 0,$$

$$r_i \leftarrow \sum_{j=1}^{n} a_{ij}, \qquad i = 1,\dots,n,$$

$$c_j \leftarrow \sum_{i=1}^{n} a_{ij}, \qquad j = 1,\dots,n,$$

$$\mu \leftarrow \frac{1}{n}\left(\sum_{i=1}^{n} r_i\right).$$

(2) Find indices p and q so that

$$|r_p - \mu| = \max_i |r_i - \mu|,$$

$$|c_q - \mu| = \max_j |c_j - \mu|.$$

If $|r_p - \mu| < \mu \cdot \text{tol}$ and $|c_q - \mu| < \mu \cdot \text{tol}$ go to step 6. If $|r_p - \mu| < |c_q - \mu|$ go to step 4.

(3) If $p = \text{lastr}$ go to step 5. Otherwise, calculate the mean $\bar{\mu}$ of row sums other than r_p:

$$\bar{\mu} \leftarrow \frac{1}{n-1}\left(\sum_{\substack{i=1\\ i\neq p}}^{n} r_i\right)$$

and scale row p to $\bar{\mu}$:

$$a_{pj} \leftarrow a_{pj} \cdot \left(\frac{\bar{\mu}}{r_p}\right), \qquad j = 1,\dots,n$$

Update row and column sums for A:

$$r_p \leftarrow \bar{\mu},$$

$$c_j \leftarrow c_j + \left(\frac{\bar{\mu}}{r_p} - 1 \right) a_{pj}, \qquad j = 1, \ldots, n,$$

$$\mu \leftarrow \bar{\mu},$$

$$\text{lastr} \leftarrow p.$$

Go to step 2.

(4) If $q = \text{lastc}$ go to step 5. Otherwise, calculate the mean $\bar{\mu}$ of column sums other than c_q:

$$\bar{\mu} \leftarrow \frac{1}{n-1} \left(\sum_{\substack{j=i \\ j \neq q}}^{n} c_j \right),$$

and scale column q to $\bar{\mu}$:

$$a_{iq} \leftarrow a_{iq} \frac{\bar{\mu}}{c_q}, \qquad i = 1, \ldots, n$$

Update row and column sums:

$$c_q \leftarrow \bar{\mu},$$

$$r_i \leftarrow r_i + \left(\frac{\bar{\mu}}{c_q} - 1 \right), \qquad i = 1, \ldots, n,$$

$$\mu \leftarrow \bar{\mu},$$

$$\text{lastc} \leftarrow q.$$

Go to step 2.

(5) Balance row lastr and column lastc (for convenience let $k = \text{lastr}$ and $l = \text{lastc}$): Multiply entries in row k by

$$f = \left(\frac{c_l - a_{kl}}{r_k - a_{kl}} \right)^{1/2}:$$

$$a_{kj} \leftarrow a_{kj} f, \qquad j = 1, \ldots, n.$$

Multiply entries in column 1 by f^{-1}:

$$a_{il} \leftarrow a_{il} f^{-1}, \qquad i = 1,\ldots,n.$$

Update row and column sums:

$$r_i \leftarrow r_i + (f^{-1} - 1) a_{il}, \qquad i = 1,\ldots,n,$$

$$r_k \leftarrow \{(r_k - a_{kl})(c_l - a_{kl})\}^{1/2} + a_{kl},$$

$$c_l \leftarrow r_k,$$

$$c_j \leftarrow c_j + (f-1) a_{kj}, \qquad j = 1,\ldots,n,$$

$$\mu \leftarrow \frac{1}{n}\left(\sum_{i=1}^{n} r_i\right).$$

Go to 2.

(6) Normalize:

$$a_{ij} \leftarrow \frac{1}{\mu} a_{ij}, \qquad i,j = 1,\ldots,n.$$

Exit.

NOTATION. To simplify the descriptions of the algorithms we have omitted programming details. In particular, we have assumed that all scaling and balancing operations are carried out explicitly by modifying entries in the matrix A. In the next section, it will be convenient to assume that the iterations are carried out implicitly by changing entries in a pair of diagonal matrices D and E.

Each algorithm produces a sequence of iteration matrices which are diagonally equivalent to the starting matrix $A = A^{(0)}$:

$$\begin{aligned} A^{(k)} &= D^{(k)} A E^{(k)}, \qquad k = 1,2,\ldots, \\ D^{(k)} &= \operatorname{diag}\left(d_1^{(k)},\ldots,d_n^{(k)}\right), \\ E^{(k)} &= \operatorname{diag}\left(e_1^{(k)},\ldots,e_n^{(k)}\right), \end{aligned} \tag{2.1}$$

and we set $D^{(0)} = E^{(0)} = I$.

We introduce the following notation:

$$A^{(k)} = \left(a_{ij}^{(k)}\right)$$

(so, for example, $a_{ij}^{(k)} = d_i^{(k)} a_{ij} e_j^{(k)}$),

$$r_i^{(k)} = \sum_{j=1}^{n} a_{ij}^{(k)}, \qquad c_j^{(k)} = \sum_{i=1}^{n} a_{ij}^{(k)}, \tag{2.2}$$

and

$$\mu_k = \frac{1}{n}\left(\sum_{i=1}^{n} r_i^{(k)}\right). \tag{2.3}$$

3. CONVERGENCE

In this section, we prove that when a starting matrix has total support, each of the algorithms described in Section 2 produces a sequence of iteration matrices which converges to a diagonally equivalent, doubly stochastic limit.

Sinkhorn and Knopp [18] showed that when SK is applied to an $n \times n$ nonnegative starting matrix $A^{(0)} = A$ possessing nonzero row and column sums, the result is a sequence of iteration matrices as in (2.1) with the following properties:

(P1) The sequence $(s_k)_{k=1,2,\dots}$ is monotonically increasing, where

$$s_k = \prod_{i=1}^{n} d_i^{(k)} e_i^{(k)}, \qquad k = 1, 2, \dots . \tag{3.1}$$

(P2) If

$$\lim_{k\to\infty} \frac{s_k}{s_{k+1}} = 1$$

then for $i, j = 1, \ldots, n$:

$$\lim_{k \to \infty} r_i^{(k)} = 1,$$

$$\lim_{k \to \infty} \frac{d_i^{(k+1)}}{d_i^{(k)}} = 1,$$

$$\lim_{k \to \infty} c_j^{(k)} = 1,$$

$$\lim_{k \to \infty} \frac{e_j^{(k+1)}}{e_j^{(k)}} = 1.$$

(P3) With the kth mean of row sums, μ_k, defined by (2.3),

$$\mu_k = 1, \qquad k = 1, 2, \ldots .$$

Algorithms which, given an $n \times n$ nonnegative starting matrix A, produce a sequence of iteration matrices as in (2.1) satisfying (P1), (P2), and (P3) will be called *diagonal product increasing* (DPI). The following result is a simple generalization of the convergence theorem in [18].

THEOREM 1. *Given a sequence* (2.1) *of diagonal equivalents for* A *satisfying* (P1), (P2), *and* (P3):

(1) *If* A *has support, then* $\lim_{k \to \infty} A^{(k)}$ *exists and is doubly stochastic.*

(2) *If* A *has total support, then the limit in* (1) *is diagonally equivalent to* A.

Before proving the theorem we state and prove a corollary:

COROLLARY.

(1) *If* A *is diagonally equivalent to a doubly stochastic matrix,* S, *then*

$$S = \lim_{k \to \infty} A^{(k)}.$$

(2) *If* A *has support and is not diagonally equivalent to a doubly stochastic matrix, then for each pair of indices* (i, j) *such that* a_{ij} *does not lie on a positive diagonal,*

$$\lim_{k \to \infty} a_{ij}^{(k)} = 0.$$

Proof of Corollary. (1): By Birkhoff's theorem [3] the set of $n \times n$ doubly stochastic matrices is the convex hull of the set of $n \times n$ permutation matrices. Therefore, S and its diagonal equivalent A have total support. Now the theorem implies that $\lim_{k\to\infty} A^{(k)}$ is doubly stochastic and diagonally equivalent to A. Since doubly stochastic equivalents are unique [19],

$$\lim_{k\to\infty} A^{(k)} = S.$$

(2): By the theorem, $\lim_{k\to\infty} A^{(k)}$ is doubly stochastic, so it has total support, and $\lim_{k\to\infty} a_{ij}^{(k)} = 0$ whenever a_{ij} does not lie on a positive diagonal. ∎

Note that matrices without support are not covered by the preceding theorem or its corollary. Such matrices are always singular, and V. Kahan (private communication), has shown that the sequence of iteration matrices $(A^{(k)})$ produced by SK cycles for such a starting matrix.

Proof of Theorem 1. We shall need the following well-known result:

LEMMA 1 (The arithmetic–geometric-mean inequality). *If $x_i \geqslant 0$ for $i = 1,\dots,n$ then*

$$\prod_{i=1}^{n} x_i \leqslant \left(\sum_{i=1}^{n} x_i/n \right)^n$$

with equality only when $x_1 = x_2 = \cdots = x_n$.

(1): (P1) implies $(s_k)_{k=1,2,\dots}$ is monotonically increasing. Since A has support, a permutation σ of $\{1,\dots,n\}$ exists such that

$$\{a_{i,\sigma(i)} | i = 1,\dots,n\}$$

is a positive diagonal in A. Let $a = \min_i(a_{i,\sigma(i)})$. Then

$$\sum_{i=1}^{n} d_i^{(k)} e_{\sigma(i)}^{(k)} a \leqslant \sum_{i=1}^{n} d_i^{(k)} e_{\sigma(i)}^{(k)} a_{i,\sigma(i)} = \sum_{i=1}^{n} a_{i\sigma(i)}^{(k)} \leqslant \sum_{i=1}^{n} r_i^{(k)} = n.$$

[Property (P3) is used for the right-hand equality.] By the arithmetic geometric inequality,

$$s_k = \prod_{i=1}^{n} d_i^{(k)} e_{\sigma(i)}^{(k)} \leqslant a^{-n}$$

and $(s_k)_{k=1,2,\ldots}$ is bounded. Therefore by (P1)

$$\lim_{k\to\infty} s_k = L > 0$$

exists, and

$$\lim_{k\to\infty} \frac{s_k}{s_{k+1}} = 1.$$

By (P2),

$$\lim_{k\to\infty} \frac{d_i^{(k+1)}}{d_i^{(k)}} = 1 \quad \text{and} \quad \lim_{k\to\infty} \frac{e_j^{(k+1)}}{e_j^{(k)}} = 1.$$

By (P3), since the $A^{(k)}$ are nonnegative, no entry $a_{ij}^{(k)}$ can be larger than n. Therefore, for each index pair (i, j) the sequence $(a_{ij}^{(k)})$ is Cauchy, and

$$\lim_{k\to\infty} A^{(k)} = A^{(\infty)}$$

exists. Since the row and column sums in $A^{(\infty)}$ must be

$$\lim_{k\to\infty} r_i^{(k)} = r_i^{(\infty)}, \qquad i = 1,\ldots,n,$$

$$\lim_{k\to\infty} c_j^{(k)} = c_j^{(\infty)}, \qquad j = 1,\ldots,n,$$

(P2) implies that $A^{(\infty)}$ is doubly stochastic.

(2): To prove the second half of the theorem we will need the following lemma, which is paraphrased from [18, p. 345].

LEMMA 2. *If A is a nonnegative matrix with total support, $(x_i^{(k)})$ and $(y_i^{(k)})$ are positive sequences for $i = 1,\ldots,n$ and $j = 1,\ldots,n$, and*

$$\lim_{k\to\infty} x_i^{(k)} y_j^{(k)} = L_{ij} > 0$$

for each index pair (i, j) such that $a_{ij} \neq 0$, then there exist positive sequences $(\bar{x}_i^{(k)})$ and $(\bar{y}_j^{(k)})$ with positive limits such that:

$$\bar{x}_i^{(k)} \bar{y}_j^{(k)} = x_i^{(k)} y_j^{(k)} \qquad \text{for all } i, j, \text{ and } k.$$

Now for the proof. From part (1), we know that $\lim_{k\to\infty} a_{ij}^{(k)} = \lim_{k\to\infty} d_i^{(k)} e_j^{(k)} a_{ij}$ exists for any i and j. If $a_{ij} \neq 0$, then $\lim_{k\to\infty} d_i^{(k)} e_j^{(k)}$ exists. Using (P1), we show that this limit is positive.

If $a_{ij} \neq 0$, it lies on a positive diagonal in A, because A has total support. Let σ be a permutation of $\{1,\dots,n\}$ such that

$$\sigma(i) = j,$$

$$a_{l\sigma(l)} > 0, \qquad l = 1,\dots,n.$$

By (P1),

$$d_i^{(k)} e_j^{(k)} \prod_{\substack{l=1\\ l\neq i}}^{n} d_l^{(k)} e_{\sigma(l)}^{(k)} = s_k \geqslant s_1, \qquad k = 1,2,\dots,$$

$$d_i^{(k)} e_j^{(k)} \geqslant s_1 \left(\prod_{\substack{l=1\\ l\neq i}}^{n} d_l^{(k)} e_{\sigma(l)}^{(k)} \right)^{-1}, \qquad k = 1,2,\dots. \tag{3.2}$$

Let $a = \min_{i,j}\{a_{ij} | a_{ij} \neq 0\}$. Then

$$a\left(\sum_{\substack{l=1\\ l\neq i}}^{n} d_l^{(k)} e_{\sigma(l)}^{(k)} \right) \leqslant \sum_{\substack{l=1\\ l\neq i}}^{n} d_l^{(k)} e_{\sigma(l)}^{(k)} a_{l,\sigma(l)} \leqslant \sum_{i=1}^{n} r_i^{(k)} = n,$$

$$\frac{a\left(\sum_{\substack{l=1\\ l\neq i}}^{n} d_l^{(k)} e_{\sigma(l)}^{(k)} \right)}{n-1} \leqslant \frac{n}{n-1}.$$

Now apply the arithmetic–geometric-mean inequality:

$$\prod_{\substack{l=1\\ l\neq i}}^{n} d_l^{(k)} e_{\sigma(l)}^{(k)} \leqslant \left(\frac{na^{-1}}{n-1} \right)^{n-1},$$

or

$$\left(\prod_{\substack{l=1\\ l\neq i}}^{n} d_l^{(k)} e_{\sigma(l)}^{(k)} \right)^{-1} \geqslant \left(\frac{(n-1)a}{n} \right)^{n-1}. \tag{3.3}$$

Combining (3.2) and (3.3),

$$d_i^{(k)}e_j^{(k)} \geqslant s_i\left(\frac{(n-1)a}{n}\right)^{n-1} > 0, \tag{3.4}$$

which shows that $\lim_{k\to\infty} d_i^{(k)}e_j^{(k)} > 0$ whenever $a_{ij} \neq 0$. Now we can apply Lemma 2 to see that positive sequences $(\bar{d}_i^{(k)})$ and $(\bar{e}_j^{(k)})$ with positive limits exist such that

$$\bar{d}_i^{(k)}\bar{e}_j^{(k)} = d_i^{(k)}e_j^{(k)} \qquad \text{for each } i, j, \text{ and } k.$$

Set

$$\bar{D}^{(k)} = \operatorname{diag}\left(\bar{d}_i^{(k)}\right)$$

and

$$\bar{E}^{(k)} = \operatorname{diag}\left(\bar{e}_i^{(k)}\right).$$

Then

$$\lim_{k\to\infty} \bar{D}^{(k)} = \bar{D}^{(\infty)} \quad \text{and} \quad \lim_{k\to\infty} \bar{E}^{(k)} = \bar{E}^{(\infty)}$$

exist. Taking limits on both sides of

$$\bar{D}^{(k)}A\bar{E}^{(k)} = A^{(k)},$$

we obtain

$$D^{(\infty)}AE^{(\infty)} = A^{(\infty)}. \qquad \blacksquare$$

Naturally, the Sinkhorn-Knopp method is product increasing; in the next theorem, we will show that normalized versions of DEV, BAL, and EQ are too. Here is another example of a DPI algorithm defined for irreducible, nonnegative matrices:

ALGORITHM. At each step: Normalize the rows by finding Y, a positive diagonal matrix, so that $YA^{(k)}$ has row sums 1. Then normalize the columns by a diagonal similarity transform defined as follows: Let $x=(x_1,\dots,x_n)$ be a left Perron vector for $YA^{(k)}$:

$$xYA^{(k)}=1\cdot x,$$

and let $X=\operatorname{diag}(x_1,\dots,x_n)$. Then

$$A^{(k+1)}=(XY)A^{(k)}X^{-1}$$

has column sums 1 because

$$(1,\dots,1)A^{(k+1)}=(1,\dots,1).$$

(Note that the similarity transform leaves diagonal products unchanged.)

Next we apply Theorem 1 to show that the algorithms described in Section 2 are convergent for starting matrices with total support.

THEOREM 2. *Suppose that the sequence of iteration matrices*

$$A^{(k)}=D^{(k)}AE^{(k)},\qquad k=1,\dots,n,$$

results from the application of DEV, BAL, *or* EQ *to* $A=A^{(0)}$; *then if* A *has total support*, $\lim_{k\to\infty}A^{(k)}/\mu_k$ *is doubly stochastic and diagonally equivalent to* A.

Proof. We prove Theorem 2 by showing that the sequence of normalized iteration matrices

$$\overline{A}^{(k)}=\frac{A^{(k)}}{\mu_k}=\overline{D}^{(k)}AE^{(k)}=\left(\frac{1}{\mu_k}D^{(k)}\right)AE^{(k)},\qquad k=1,2,\dots,\tag{3.5}$$

satisfies (P1), (P2), and (P3).

(P3) is obviously satisfied by (3.5). Note that

$$\begin{aligned}s_k&=\prod_{i=1}^{n}\left(\frac{1}{\mu_k}d_i^{(k)}\right)e_i^{(k)}\\&=\frac{1}{\mu_k^n}\prod_{i=1}^{n}d_i^{(k)}e_i^{(k)},\qquad k=1,2,\dots.\end{aligned}$$

DEV: Suppose that at step $k+1$ row p is scaled to the mean of the other row sums, $\bar{\mu}$. After the scaling, $\bar{\mu}$ is the mean of row sums, that is,

$$\bar{\mu} = \mu_{k+1},$$

and in this case

$$\begin{aligned}
\frac{s_{k+1}}{s_k} &= \left(\frac{1/\mu_{k+1}}{1/\mu_k}\right)^n \frac{\prod_{i=1}^{n} d_i^{(k+1)} e_i^{(k+1)}}{\prod_{i=1}^{n} d_i^{(k)} e_i^{(k)}} \\
&= \left(\frac{1/\mu_{k+1}}{1/\mu_k}\right)^n \frac{\mu_{k+1}}{r_p} \\
&= \left(\frac{\mu_k}{\mu_{k+1}}\right)^{n-1} \frac{\mu_k}{r_p}.
\end{aligned} \tag{3.6}$$

Since μ_{k+1} is the mean of row sums other than r_p in $A^{(k)}$, and μ_k is the mean of all row sums,

$$\begin{gathered}
\frac{r_p + (n-1)\mu_{k+1}}{n} = \mu_k, \\
\frac{1}{n}\left(\frac{r_p}{\mu_k} + \frac{(n-1)\mu_{k+1}}{\mu_k}\right) = 1
\end{gathered} \tag{3.7}$$

By the arithmetic–geometric-mean inequality

$$\frac{r_p \mu_{k+1}^{n-1}}{\mu_k^n} \leqslant 1.$$

Therefore

$$\frac{s_{k+1}}{s_k} = \left(\frac{\mu_k}{\mu_{k+1}}\right)^{n-1} \frac{\mu_k}{r_p} \geqslant 1.$$

The above argument can be repeated for a column scaling at step $k+1$, and

(P1) holds. Next define sequences

$$\left(x_i^{(k)}\right)_{k=1,2,\dots}, \qquad i=1,\dots,n, \tag{3.8}$$

by

$$x_i^{(k+1)} = \begin{cases} r_p/\mu_k & \text{if } \ i=p \text{ and at step } (k+1) \text{ row } p \text{ is scaled} \\ & \qquad \text{to the mean of the other row sums,} \\ c_q/\mu_k & \text{if } \ i=q \text{ and at step } (k+1) \text{ column } q \text{ is scaled} \\ & \qquad \text{to the mean of the other column sums,} \\ \mu_{k+1}/\mu_k & \text{otherwise.} \end{cases}$$

By (3.7), $(1/n)\Sigma_{i=1}^n x_i^{(k)} = 1$ for each k. Using the arithmetic–geometric-mean inequality, it can be shown that from

$$\lim_{k\to\infty} \prod x_i^{(k+1)} = \lim_{k\to\infty} \frac{s_{k+1}}{s_k} = 1$$

follows

$$\lim_{k\to\infty} x_i^{(k)} = 1, \qquad i=1,\dots,n.$$

Since

$$\frac{\bar{d}_i^{(k+1)}}{\bar{d}_i^{(k)}} = \frac{\mu_k}{\mu_{k+1}} \ \text{ or } \ \frac{\bar{d}_i^{(k+1)}}{\bar{d}_i^{(k)}} = \frac{\mu_{k+1}}{r_p}\frac{\mu_k}{\mu_{k+1}} = \frac{\mu_k}{r_p}, \qquad i=1,\dots,n,$$

and

$$\frac{\bar{d}_i^{(k+1)}}{\bar{d}_i^{(k)}} = \frac{1}{x_l^{(k+1)}} \qquad \text{for some } l,$$

and similarly

$$\frac{e_i^{(k+1)}}{e_i^{(k)}} = 1 \text{ or } \frac{\mu_k}{c_q}, \qquad i=1,\dots,n,$$

$$= 1 \text{ or } \frac{1}{x_l^{(k+1)}} \qquad \text{for some } l,$$

it follows that

$$\lim_{k\to\infty}\frac{\bar{d}_i^{(k+1)}}{\bar{d}_i^{(k)}}=\lim_{k\to\infty}\frac{e_i^{(k+1)}}{e_i^{(k)}}=1,\qquad i=1,\dots,n.$$

At each step, DEV selects p or q so that

$$\left|\frac{r_p}{\mu_k}-1\right| \quad\text{or}\quad \left|\frac{c_q}{\mu_k}-1\right|$$

is maximal. It follows that for $i,j=1,\dots,n$

$$\lim_{k\to\infty}\frac{r_i^{(k)}}{\mu_k}=\lim_{k\to\infty}\frac{c_j^{(k)}}{\mu_k}=1.$$

Therefore (P2) holds for the sequence (3.5) produced by DEV.

BAL: Suppose that at step $k+1$ BAL balances row p and column q. Let

$$x^{(k)}=r_p^{(k)}-a_{pq}^{(k)},$$

$$y^{(k)}=c_q^{(k)}-a_{pq}^{(k)}.$$

In this case

$$\frac{s_{k+1}}{s_k}=\left(\frac{1/\mu_{k+1}}{1/\mu_k}\right)^n\cdot f\cdot f^{-1}=\left(\frac{\mu_k}{\mu_{k+1}}\right)^n, \tag{3.9}$$

where

$$f=\left(\frac{x^{(k)}}{y^{(k)}}\right)^{1/2},$$

so to show that $s_{k+1}\geqslant s_k$, we must show that $\mu_{k+1}\leqslant\mu_k$.

If $A^{(k)}$ is doubly stochastic for some k, then $A^{(k)}=A^{(k+1)}=\cdots$ and the theorem is satisfied. Otherwise, for each k, we may assume that

$$\left|r_p^{(k)}-c_q^{(k)}\right|=\left|x^{(k)}-y^{(k)}\right|\neq 0. \tag{3.10}$$

With this assumption, if $x^{(k)}=0$ or $y^{(k)}=0$, then A cannot have total support—a contradiction. Therefore, $x^{(k)}\neq 0$ and $y^{(k)}\neq 0$, and the denominators for f and f^{-1} are never 0.

The entries in $A^{(k)}$ sum to

$$\sum_{i=1}^{n} r_i^{(k)} = \sum_{i,j=1}^{n} a_{ij}^{(k)}$$

$$= \left(\sum_{\substack{i,j=1\\ i\neq p\\ j\neq q}}^{n} a_{ij}^{(k)} \right) + x^{(k)} + y^{(k)} + 2a_{pq}^{(k)}. \tag{3.11}$$

After the balancing step, the entries in $A^{(k+1)}$ sum to

$$\sum_{i=1}^{n} r_i^{(k+1)} = \left(\sum_{\substack{i=1\\ i\neq p\\ i\neq q}}^{n} a_{ij}^{(k)} \right) + 2\left(x^{(k)}y^{(k)}\right)^{1/2} + 2a_{pq}^{(k)}, \tag{3.12}$$

so

$$\mu_{k+1} = \frac{\sum_{i=1}^{n} r_i^{(k+1)}}{n}$$

$$= \frac{\sum_{i=1}^{n} r_i^{(k)} + \left[2\sqrt{x^{(k)}y^{(k)}} - \left(x^{(k)}+y^{(k)}\right)\right]}{n}$$

$$= \mu_k + \frac{2\sqrt{x^{(k)}y^{(k)}} - \left(x^{(k)}+y^{(k)}\right)}{n} \tag{3.13}$$

By the arithmetic–geometric-mean inequality

$$2\sqrt{x^{(k)}y^{(k)}} \leqslant x^{(k)} + y^{(k)},$$

and therefore

$$\mu_{k+1} \leqslant \mu_k. \tag{3.14}$$

By (3.9), $s_{k+1}/s_k = (\mu_k/\mu_{k+1})^n \geqslant 1$ and $s_{k+1} \geqslant s_k$, i.e., (P1) is satisfied.

Suppose that

$$\lim_{k\to\infty} \frac{s_{k+1}}{s_k} = 1. \tag{3.15}$$

Then by (3.9) and (3.13),

$$1 = \lim_{k\to\infty} \frac{\mu_k}{\dfrac{\mu_k + 2\sqrt{x^{(k)}y^{(k)}} - \left(x^{(k)} + y^{(k)}\right)}{n}}$$

$$= \lim_{k\to\infty} \frac{\mu_k}{\dfrac{(n\cdot\mu_k) + 2\sqrt{x^{(k)}y^{(k)}} - \left(x^{(k)} + y^{(k)}\right)}{n}}$$

$$= \lim_{k\to\infty} \frac{1}{1 + \dfrac{2\sqrt{x^{(k)}y^{(k)}} - \left(x^{(k)} + y^{(k)}\right)}{n\mu_k}}, \tag{3.16}$$

which implies that

$$\lim_{k\to\infty} \frac{2\sqrt{x^{(k)}y^{(k)}} - x^{(k)} + y^{(k)}}{n\mu_k} = 0,$$

$$\lim_{k\to\infty} \left[2\sqrt{\frac{x^{(k)}}{\mu_k}\frac{y^{(k)}}{\mu_k}} - \left(\frac{x^{(k)}}{\mu_k} + \frac{y^{(k)}}{\mu_k}\right)\right] = 0.$$

It follows from the arithmetic–geometric-mean inequality that this is impossible unless

$$\lim_{k\to\infty} \frac{x^{(k)}}{\mu_k} - \frac{y^{(k)}}{\mu_k} = 0$$

and

$$\lim_{k\to\infty} \left(\max_{i,j} \left|\frac{r_i^{(k)}}{\mu_k} - \frac{c_j^{(k)}}{\mu_k}\right|\right) = 0.$$

The mean of the row sums and the mean of the column sums in $A^{(k)}/\mu_k$ is 1, implying

$$\lim_{k\to\infty} \frac{r_i^{(k)}}{\mu_k} = \lim_{k\to\infty} \frac{c_j^{(k)}}{\mu_k} = 1.$$

Equation (3.4) in the proof of Theorem 1 holds whenever (P1) and (P3) are satisfied, and for each index pair (i, j) such that $a_{ij} \neq 0$, the sequence

$$\left(\frac{a_{ij}^{(k)}}{\mu_k}\right)_{k=1,2,\ldots}$$

is bounded away from zero. Therefore, the sequences $(x^{(k)}/\mu_k)$ and $(y^{(k)}/\mu_k)$ are bounded away from zero, because $x^{(k)} \neq 0$ and $y^{(k)} \neq 0$ for each k. We have

$$\lim_{k\to\infty} \frac{x^{(k)}/\mu_k}{y^{(k)}/\mu_k} = \lim_{k\to\infty} \frac{x^{(k)}}{y^{(k)}} = 1. \tag{3.17}$$

Finally, for each i, j, and k,

$$\frac{\bar{d}_i^{(k+1)}}{\bar{d}_i^{(k)}} = \frac{\mu_k}{\mu_{k+1}} \frac{d_i^{(k+1)}}{d_i^{(k)}} = \frac{\mu_k}{\mu_{k+1}} \quad \text{or} \quad \frac{\bar{d}_i^{(k+1)}}{\bar{d}_i^{(k)}} = \frac{\mu_k}{\mu_{k+1}} \left(\frac{y^{(k)}}{x^{(k)}}\right)^{1/2},$$

$$\frac{e_j^{(k+1)}}{e_j^{(k)}} = 1 \quad \text{or} \quad \frac{e_j^{(k+1)}}{e_j^{(k)}} = \left(\frac{x^{(k)}}{y^{(k)}}\right)^{1/2}.$$

Therefore, by (3.15) and (3.17),

$$\lim_{k\to\infty} \frac{\bar{d}_i^{(k+1)}}{\bar{d}_i^{(k)}} = \lim_{k\to\infty} \frac{e_j^{(k+1)}}{e_j^{(k)}} = 1 \tag{3.18}$$

for each i, and j, and (P2) is satisfied.

EQ: Each step of EQ is a step of DEV or a balancing step. The arguments above for DEV and BAL show that for each k, $s_{k+1} \geqslant s_k$, i.e. that (P1) holds. Consider the sequence (3.8) and its subsequence

$$\left(x_i^{(k)}\right)_{k'=p_1,p_2,\ldots},$$

where at steps $k' = p_1, p_2, \ldots$ EQ scaled a row or column to the mean of the other row or column sums. This sequence must be infinite—because lastr and lastc are set to 0 after each balancing step—and the argument for DEV can be repeated to show that for $i, j = 1, \ldots, n$,

$$\lim_{k'\to\infty} \frac{\bar{d}_i^{(k'+1)}}{\bar{d}_i^{(k')}} = 1,$$

$$\lim_{k'\to\infty} \frac{e_i^{(k'+1)}}{e_i^{k'}} = 1,$$

$$\lim_{k'\to\infty} \frac{r_i^{k'}}{\mu_{k'}} = 1, \tag{3.19}$$

$$\lim_{k'\to\infty} \frac{c_j^{k'}}{\mu_{k'}} = 1.$$

Next consider the subsequence

$$\left(x_i^{(k'')}\right)_{k''=q_1,q_2,\ldots},$$

where at steps $k'' = q_1, q_2, \ldots$ EQ balanced a row and column. If this sequence is infinite, the arguments for BAL [Equations (3.15)–(3.18)] can be repeated to show that when $\lim_{k\to\infty}(s_{k+1}/s_k) = 1$,

$$\lim_{k''\to\infty} \frac{\bar{d}_i^{(k''+1)}}{\bar{d}_i^{(k'')}} = 1, \tag{3.20}$$

$$\lim_{k''\to\infty} \frac{e_i^{(k'')}}{e_i^{(k'')}} = 1.$$

(3.19) and (3.20) imply that

$$\lim_{k\to\infty} \frac{\bar{d}_i^{(k+1)}}{\bar{d}_i^{(k)}} = \lim_{k\to\infty} \frac{e_i^{(k+1)}}{e_i^{(k)}} = 1.$$

In particular, $\lim_{k\to\infty} A^{(k)}$ exists, and its row and column sums are

$$\lim_{k\to\infty} \frac{r_i^{(k)}}{\mu_k} = \lim_{k'\to\infty} \frac{r_i^{(k')}}{\mu'_k} = 1,$$

$$\lim_{k\to\infty} \frac{c_j^{(k)}}{\mu_{(k)}} = \lim_{k'\to\infty} \frac{c_j^{(k')}}{\mu_{k'}} = 1.$$

(P3) holds for the sequence (3.5) produced by EQ. ■

It is possible to show that each of the sequences $(d_i^{(k)})$ and $(e_j^{(k)})$, $i, j = 1,\dots,n$, produced by SK and BAL is Cauchy. We believe the same to be true for DEV and EQ but are unable to prove it.

4. TEST RESULTS

We ran comparison tests of the algorithms described in this paper and the Sinkhorn-Knopp method on a thoughtful collection of 50 10×10 or smaller matrices. These tests were run on a VAX 11/780 at U.C. Berkeley, with 7 significant digits in single precision and 16 digits in double precision. Sums were accumulated in double precision.

For convergence to "tol" accuracy, we required that all row and column sums deviate from the mean μ by less than $\text{tol}\cdot\mu$. So, in the normalized matrices, row and column sums could not deviate from 1 by more than tol.

The examples selected for this section illustrate the following points:

(1) EQ exhibited significantly better average and worst-case behavior than SK on our test bed. For convergence to $\text{tol} = 10^{-5}$, the ratio of total SK operations to total EQ operations varied from a low of $\frac{1}{2}$ to a high of more than 130.

(2) We found striking examples where EQ was significantly faster than DEV, BAL, or SK (see H_5 below). Since each iteration by EQ scaled a row or column (like DEV) or balanced a row and column pair (like BAL), there is evidence that some mechanism is at work which enables EQ to choose the right operation at the right time.

These first four examples were the test matrices in [10]:

$$A = \begin{pmatrix} 10^4 & 10^2 & 10^2 \\ 10^2 & 1 & 1 \\ 10^2 & 1 & 1 \end{pmatrix}, \qquad B = \begin{pmatrix} 10^2 & 1 & 0 \\ 10^2 & 10^3 & 1 \\ 0 & 10^2 & 10^2 \end{pmatrix},$$

$$C=\begin{pmatrix} 10^2 & 10^2 & 0 \\ 10^2 & 10^4 & 1 \\ 0 & 1 & 10^2 \end{pmatrix}, \qquad D=\begin{pmatrix} 10^4 & 1 & 0 \\ 10^4 & 10^6 & 1 \\ 0 & 10^4 & 10^4 \end{pmatrix}.$$

The results are as follows (for tol $= 10^{-5}$):

Matrix	Steps to convergence: DEV	BAL	EQ	SK	SK ops / EQ ops.
A	2	32	2	1	0.9
B	402	34	46	150	6.0
C	3281	34	49	1899	71.5
D	7961	40	40	2983	137.7

Here "steps" for DEV, BAL, and EQ, were counted in the following way: each scaling of a row or column counted as one step, and each balancing of a row-column pair counted as two steps. A step for SK consisted of normalizing rows and normalizing columns.

Five other test matrices were 10×10 upper Hessenberg matrices: $H_1 = (h_{ij})$, where

$$h_{ij}=\begin{cases} 0 & \text{if } j<i-1, \\ 1 & \text{otherwise.}\end{cases}$$

H_2, H_3 and H_4 each differ from H_1 in a single entry:

the $(1,1)$ entry in H_2 is 100,
the $(1,2)$ entry in H_3 is 100,
the $(1,3)$ entry in H_4 is 100.

H_5 is the result of replacing all diagonal entries in H_1 by 100. The results are as follows (for tol $= 10^{-5}$):

Matrix	Steps to convergence: DEV	BAL	EQ	SK	SK ops. / EQ ops.
H_1	812	748	812	55	0.6
H_2	873	926	717	72	0.8
H_3	925	952	775	71	0.7
H_4	953	948	921	71	0.6
H_5	14476	17456	917	1004	8.9

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